Cross-Validation

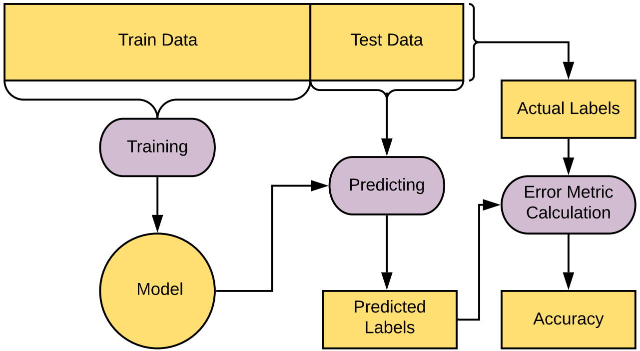
Nipun Batra and teaching staff

IIT Gandhinagar

August 2, 2025

Outline

Our General Training Flow



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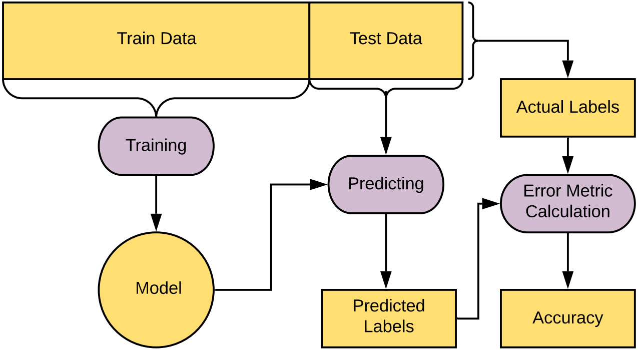

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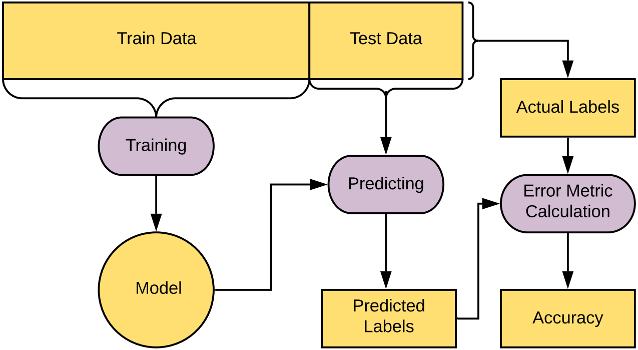

- Does not use the full dataset for training and does not test on the full dataset

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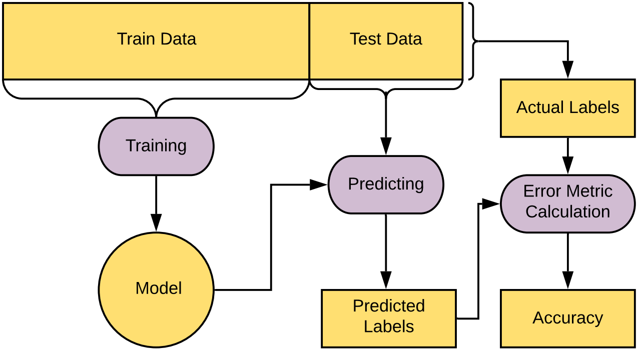

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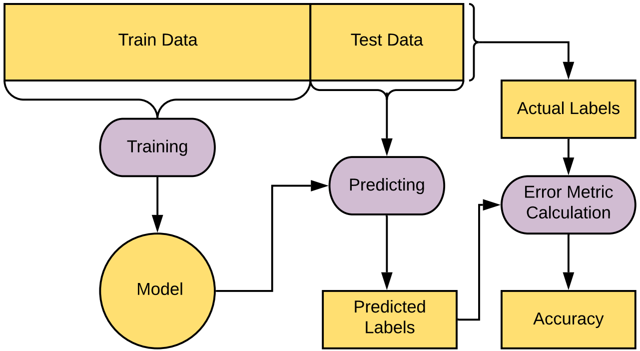

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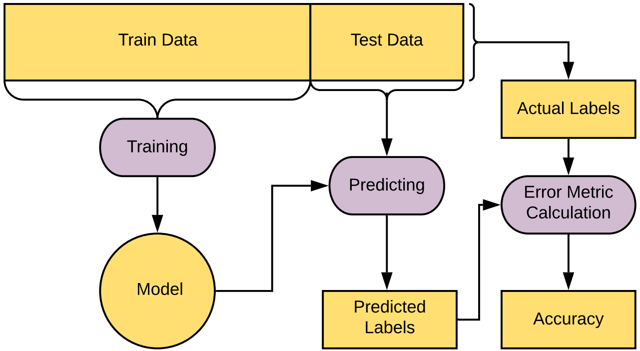

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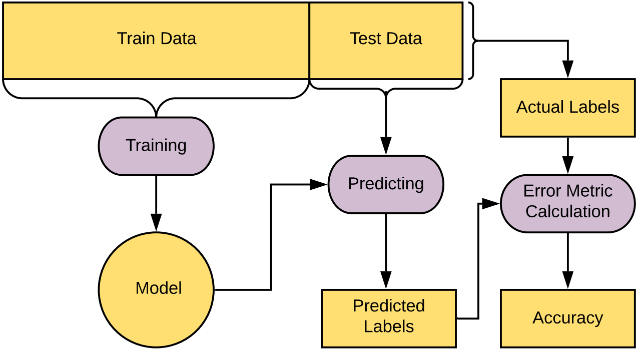

- Does not use the full dataset for training and does not test on the full dataset
- No way to optimize hyperparameters
- This simple train/test split has limitations we need to address

Pop Quiz #1

Question

What are the main limitations of using only a single train/test split?

Pop Quiz #2

Question

What are the main limitations of using only a single train/test split?

Pop Quiz #3

Question

What are the main limitations of using only a single train/test split?

Answer

Pop Quiz #4

Question

What are the main limitations of using only a single train/test split?

Answer

- Does not utilize the full dataset for training

Pop Quiz #5

Question

What are the main limitations of using only a single train/test split?

Answer

- Does not utilize the full dataset for training
- Cannot optimize hyperparameters systematically

Pop Quiz #6

Question

What are the main limitations of using only a single train/test split?

Answer

- Does not utilize the full dataset for training
- Cannot optimize hyperparameters systematically
- Results depend on the particular split chosen

Pop Quiz #7

Question

What are the main limitations of using only a single train/test split?

Answer

- Does not utilize the full dataset for training
- Cannot optimize hyperparameters systematically
- Results depend on the particular split chosen
- May not get reliable performance estimates

How to use the full dataset for training?

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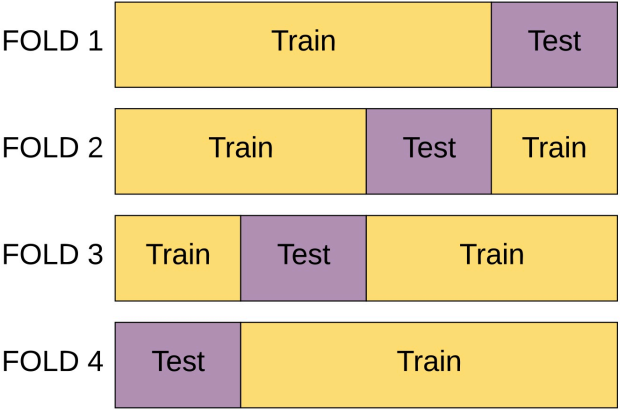
- **Challenge:** How to ensure systematic evaluation?
- May not use every data point for training or testing with random splits
- May be computationally expensive

K-Fold Cross-Validation: Utilize Full Dataset for Testing



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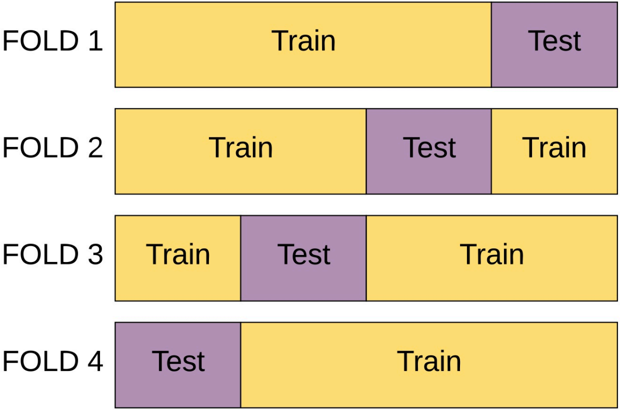

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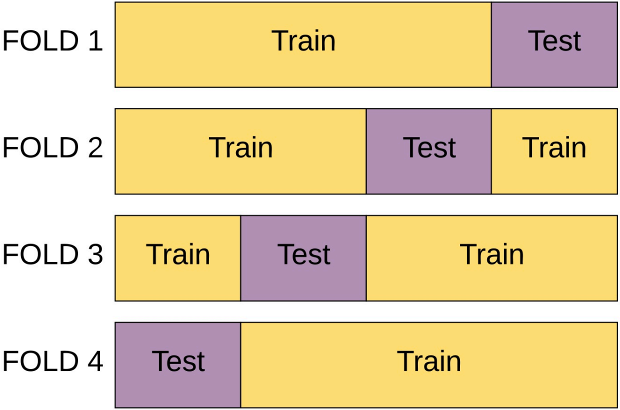

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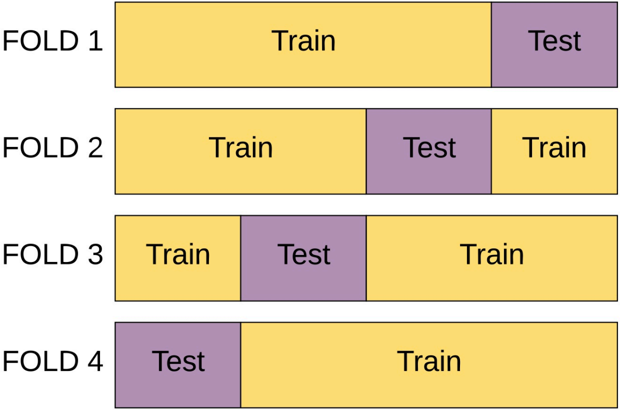

Pop Quiz #8

Question

If you have 100 data points and use 5-fold cross-validation, how many data points are used for training in each fold?

Pop Quiz #9

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Pop Quiz #10

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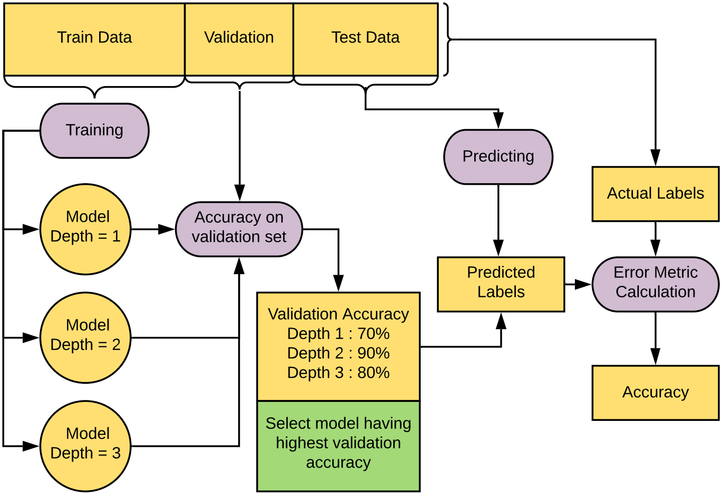
If you have 100 data points and use 5-fold cross-validation, how many data points are used for training in each fold?

Answer

80 data points (4 out of 5 folds = $4/5 \times 100 = 80$)

Optimizing Hyperparameters via the Validation Set



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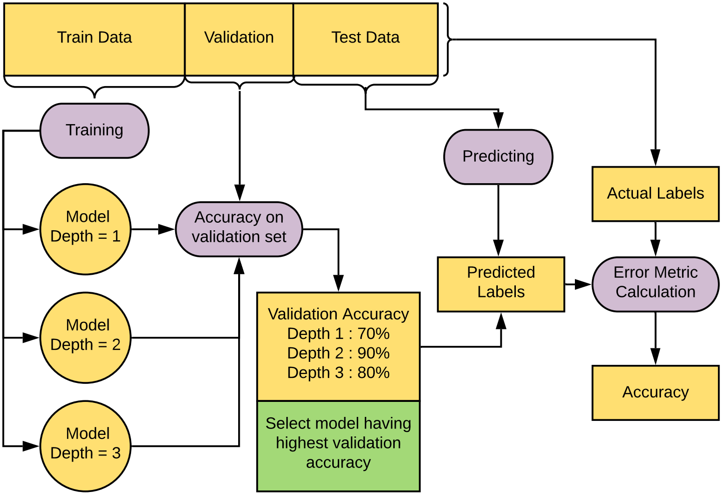

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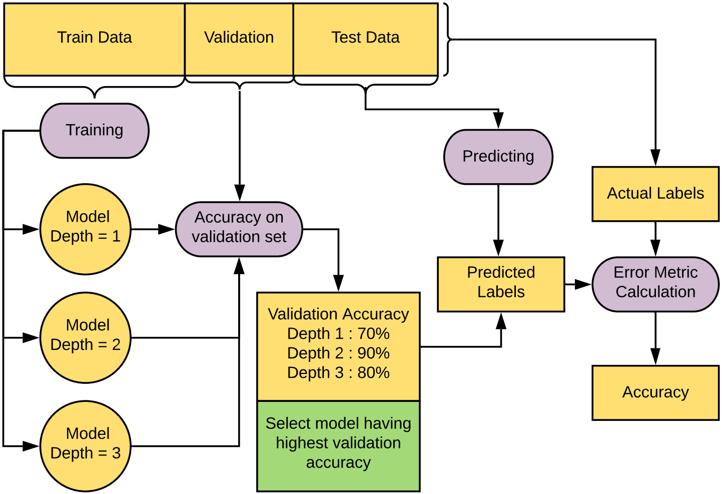

Validation set helps select the best hyperparameters

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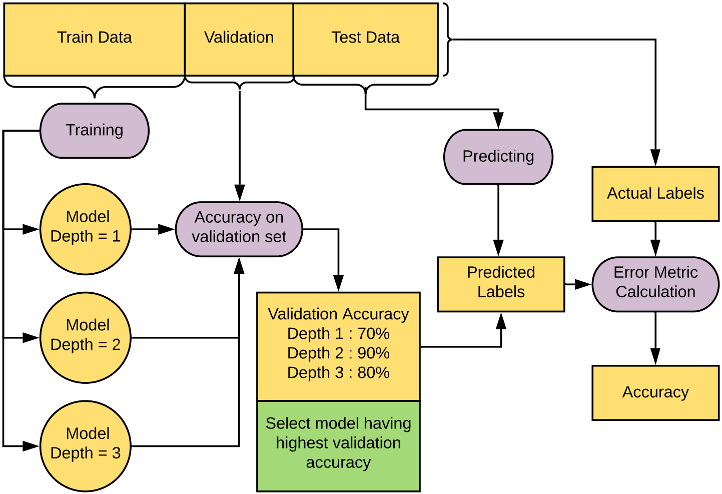

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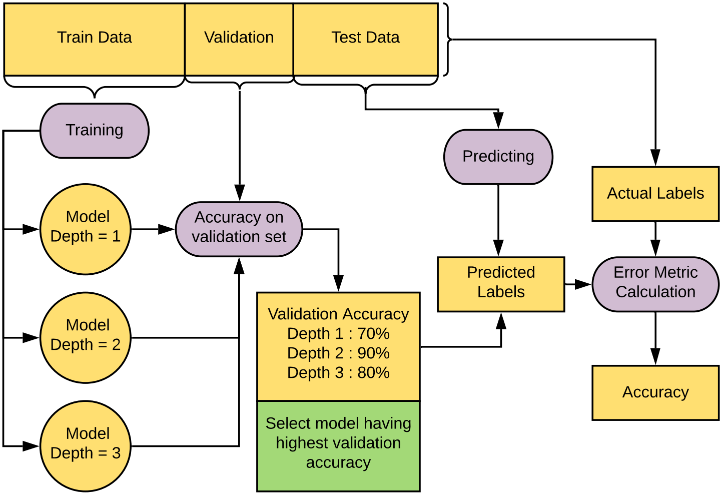

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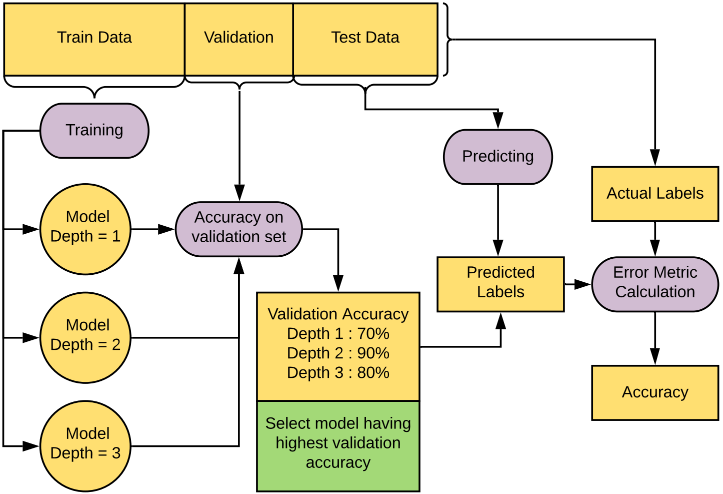

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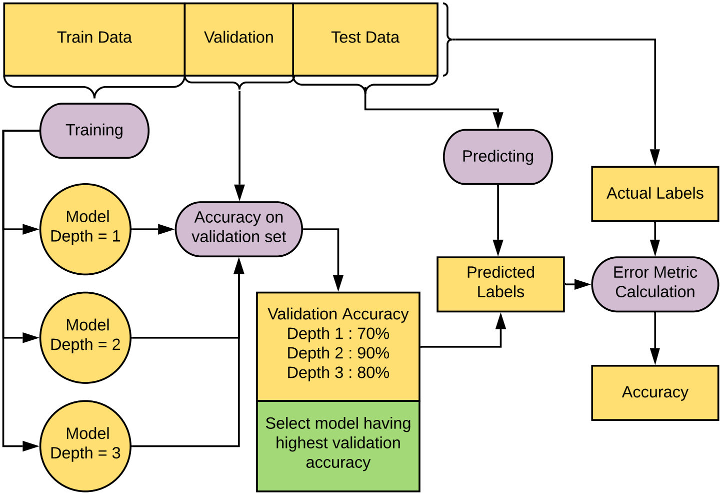
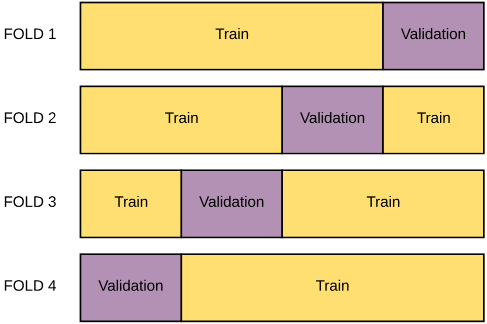


Nested Cross-Validation Process

Divide your training set into *k* equal parts.
Cyclically use 1 part as "validation set" and the rest for training.
Here $k = 4$



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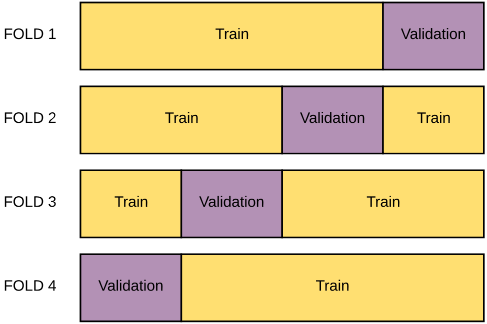

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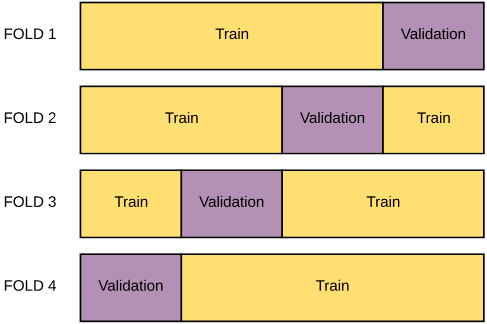

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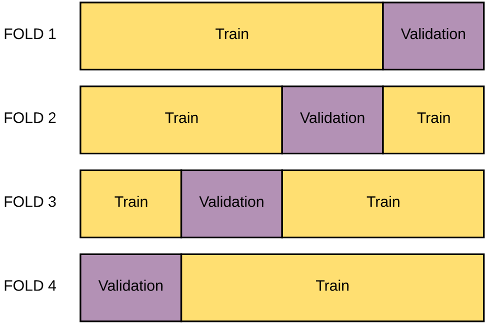

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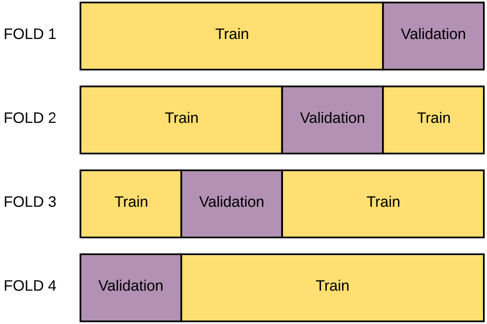

- Each fold provides one validation score
- Process is systematic and exhaustive

Pop Quiz #11

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Pop Quiz #13

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Answer

Pop Quiz #14

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Pop Quiz #15

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- Nested CV: Outer loop for model evaluation, inner loop for hyperparameter tuning

Pop Quiz #16

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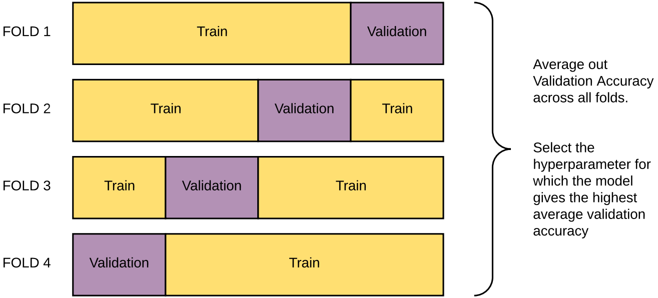
Answer

- Simple CV: Used for model evaluation only
- Nested CV: Outer loop for model evaluation, inner loop for hyperparameter tuning
- Nested CV provides unbiased estimates when doing hyperparameter search

Cross-Validation Results

- Average out the validation accuracy across all the folds
- Use the hyperparameters with highest average validation accuracy



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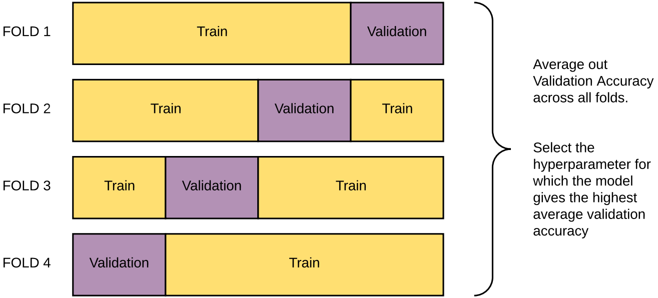

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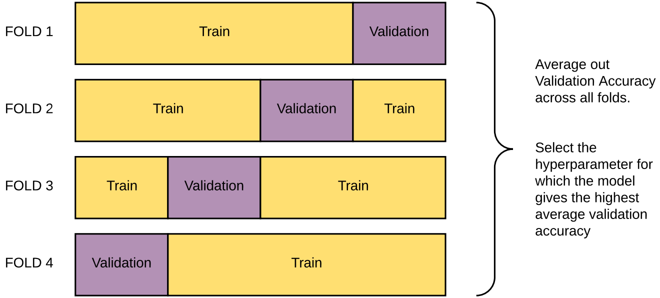

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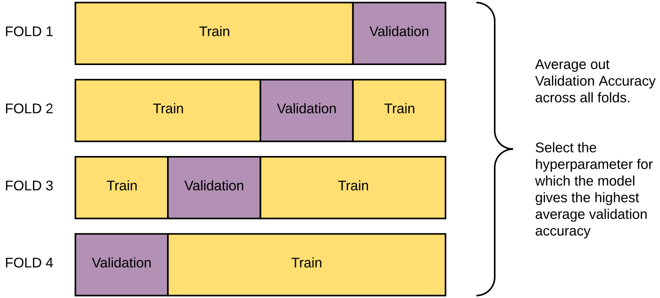

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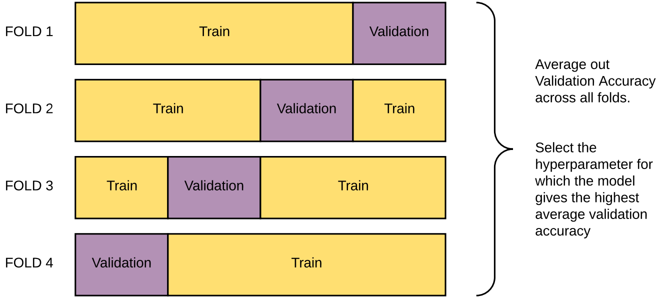

- Final model is trained on entire training set
- Standard deviation gives confidence in results

Pop Quiz #17

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Pop Quiz #18

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Pop Quiz #19

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Answer

Pop Quiz #20

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Pop Quiz #21

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- Averaging provides more robust performance estimates

Pop Quiz #22

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- Reduces impact of lucky/unlucky splits

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- Reduces impact of lucky/unlucky splits
- Standard deviation indicates reliability of the estimate

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Stratified Cross-Validation

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- Reduces variance in performance estimates

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You have a binary classification dataset with 90% negative and 10% positive examples. Why is stratified cross-validation important here?

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- Regular CV might create folds with very few (or zero) positive examples

Pop Quiz #28

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Answer

- Regular CV might create folds with very few (or zero) positive examples
- This would give misleading performance estimates
- Stratified CV ensures each fold has $\sim$10% positive examples
- Results in more reliable and consistent evaluation

Time Series Cross-Validation

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- Never use future data to predict past!

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- **Ignoring Class Imbalance:** Not using stratified CV when needed

Pop Quiz #31

Question

What's wrong with computing mean and standard deviation on the entire dataset before doing cross-validation?

Pop Quiz #32

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Pop Quiz #33

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Pop Quiz #36

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Pop Quiz #37

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- Test fold statistics influence the training preprocessing
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- Apply same transformation to corresponding test fold
- This gives more realistic performance estimates

Cross-Validation: Key Benefits

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- **Better Data Utilization:** Every point used for both training and testing

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